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Investigating the electronic and magnetic properties of Dy, Y and La by site substitution on Nd2Fe14B permanent magnet employing the first-principle approach

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Abstract

The development of new Nd-Fe-B permanent magnets continues to be a pressing matter for the transition to a green economy. Permanent magnets have become significant in applications of highly efficient energy conversion machines and devices. First-principles calculations have been performed by using the density function theory (DFT) within the generalized gradient approximation (GGA) to study the Nd2Fe14B magnets. The effects of Dy/La/Y on the electronic and magnetic properties of Nd2Fe14B permanent magnet with the site substitution mechanism were studied. The spin and the orbital magnetic moments of the Nd, Dy, Y, and La ion were found to be opposite to each other, which is in agreement with Hund's rule. Moreover, the total orbital magnetic moment was found to be larger than that of the total spin magnetic moment. Y prefers the 4f site, while La on the other hand prefers the 4g site. The total magnetic moment of the Nd2Fe14B was in close agreement with the previous reported experimental value.